Periodic Orbit Quantization of Mixed Regular-Chaotic Systems

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A general technique for the periodic orbit quantization of systems with near-integrable to mixed regular-chaotic dynamics is introduced. A small set of periodic orbits is sufficient for the construction of the semiclassical recurrence function up to, in principle, infinite length. As in our recent work the recurrence signal is inverted by means of a high resolution spectral analyzer (harmonic inversion) to obtain the semiclassical eigenenergies. The method is demonstrated for the hydrogen atom in a magnetic field. To our knowledge this is the first successful application of periodic orbit quantization in the deep mixed regular-chaotic regime.

PACS numbers: 05.45.+b, 03.65.Sq, 32.60.+i

The question of how to semiclassically quantize systems with *nonintegrable* Hamiltonians had puzzled the great minds of physics in the early days of quantum mechanics [1]. The advent of "exact" quantum mechanics, and, later, the availability of more and more powerful computing resources, with the possibility of numerically solving, in principle, Schrödinger's equation for every complex quantum system, pushed that old question in the background for several decades. However, the desire for deeper physical insight into "what the computer understands" [2] finally triggered a renaissance of semiclassical theory, which persists. It will be the objective of this Letter to contribute to solving that longstanding problem of semiclassical quantization of nonintegrable systems in the *mixed regular-chaotic* regime.

The breakthrough of modern semiclassical theory came when Gutzwiller proved, by an application of the method of stationary phase to the semiclassical approximation of the quantum propagator, that for systems with complete chaotic (hyperbolic) classical dynamics the density of states can be expressed as an infinite sum over all (isolated) periodic orbits, thus laying the foundation of periodic orbit theory [3]. Special methods were designed for specific systems to overcome the convergence problems of the semiclassical trace formula, i.e., to analytically continue its range of convergence to the physical domain [4–7]. None of these methods, however, has succeeded so far in correctly describing generic dynamical systems with mixed regular-chaotic phase spaces.

On the other extreme of complete integrability, it is well known that the semiclassical energy values can be obtained by EBK torus quantization [1]. This requires the knowledge of all the constants of motion, which are not normally given in explicit form, and therefore practical EBK quantization based on the direct or indirect numerical construction of the constants of motion turns out to be a formidable task [8]. As an alternative, EBK quantization was recast as a sum over all periodic orbits of a given topology on respective tori by Berry and Tabor [9]. The Berry-Tabor formula circumvents the numerical construction of the constants of motion but usually suffers from the convergence problems of the infinite periodic orbit sum.

The extension of the Berry-Tabor formula into the near-integrable (KAM) regime was outlined by Ozorio de Almeida [10] and elaborated, at different levels of refinement, by Tomsovic et al. and Ullmo et al. [11]. These authors noted that in the near-integrable regime, according to the Poincaré-Birkhoff theorem, two periodic orbits survive the destruction of a rational torus with similar actions, one stable and one hyperbolic unstable, and worked out the ensuing modifications of the Berry-Tabor formula. In this Letter we go one step further by noting that, with increasing perturbation, the stable orbit turns into an inverse hyperbolic one representing, together with its unstable companion with similar action, a remnant torus. We include the contributions of these pairs of inverse hyperbolic and hyperbolic orbits in the Berry-Tabor formula and demonstrate for a system with mixed regular-chaotic dynamics that this procedure yields excellent results even in the deep mixed regular-chaotic regime. The system we choose is the hydrogen atom in a magnetic field, which is a real physical system and has served extensively as a prototype for the investigation of "quantum chaos" (for reviews see [12–14]). To our knowledge no semiclassical quantization thus far in the mixed regular-chaotic region has previously been given.

The fundamental obstacle bedeviling the semiclassical quantization of systems with mixed regular-chaotic dynamics is that the periodic orbits are neither sufficiently isolated, as is required for Gutzwiller's trace formula [3], nor are they part of invariant tori, as is necessary for the Berry-Tabor formula [9]. However, as will become clear below, it is the Berry-Tabor formula which lends itself in a natural way for an extension of periodic orbit quantization to mixed systems. We consider systems with a scaling property, i.e., where the shape of periodic orbits does not depend on the scaling parameter, $w = \hbar_{\text{eff}}^{-1}$, and the classical action S scales as $S = sw$ with s the scaled action. For scaling systems with two degrees of freedom,

which we will focus on, the Berry-Tabor formula for the fluctuating part of the level density reads

$$\varrho(w) = \frac{1}{\pi} \operatorname{Re} \sum_{\mathbf{M}} \frac{w^{1/2} s_{\mathbf{M}}}{M_2^{3/2} |g_E''|^{1/2}} e^{i(s_{\mathbf{M}} w - \frac{\pi}{2} \eta_{\mathbf{M}} - \frac{\pi}{4})} , \quad (1)$$

with $\mathbf{M} = (M_1, M_2)$ pairs of integers specifying the individual periodic orbits on the tori (numbers of rotations per period, M_2/M_1 rational), and $s_{\mathbf{M}}$ and $\eta_{\mathbf{M}}$ the scaled action and Maslov index of the periodic orbit $\mathbf{M}$. The function g_E in (1) is obtained by inverting the Hamiltonian, expressed in terms of the actions (I_1, I_2) of the corresponding torus, with respect to I_2, viz. $H(I_1, I_2 = g_E(I_1)) = E$ [15]. The calculation of g_E'' from the actions (I_1, I_2) can be rather laborious even for integrable and near-integrable systems, and, by definition, becomes impossible for mixed systems in the chaotic part of the phase space. Here we will adopt the method of Ref. [11] and calculate g_E'', for given $\mathbf{M} = (\mu_1, \mu_2)$, with (μ_1, μ_2) coprime integers specifying the primitive periodic orbit, directly from the parameters of the two periodic orbits (stable (s) and hyperbolic unstable (h)) that survive the destruction of the rational torus $\mathbf{M}$, viz.

$$g_E'' = \frac{2}{\pi \mu_2^3 \Delta s} \left(\frac{1}{\sqrt{\det(M_{\mathrm{s}} - I)}} + \frac{1}{\sqrt{-\det(M_{\mathrm{h}} - I)}} \right)^{-2} , \quad (2)$$

with

$$\Delta s = \frac{1}{2}(s_{\mathrm{h}} - s_{\mathrm{s}}) \quad (3)$$

the difference of the scaled actions, and M_{s} and M_{h} the monodromy matrices of the two orbits. The action $s_{\mathbf{M}}$ in (1) is to replaced with the mean action

$$\bar{s} = \frac{1}{2}(s_{\mathrm{h}} + s_{\mathrm{s}}) . \quad (4)$$

Eq. 2 is an approximation which becomes exact in the limit of an integrable system.

It is a characteristic feature of systems with mixed regular-chaotic dynamics that with increasing nonintegrability the stable orbits turn into inverse hyperbolic unstable orbits in the chaotic part of the phase space. These orbits, although embedded in the fully chaotic part of phase space, are remnants of broken tori. It is therefore natural to assume that Eqs. 1 and 2 can even be applied when these pairs of inverse hyperbolic and hyperbolic orbits are taken into account, i.e., more deeply in the mixed regular-chaotic regime.

It should be noted that the difference Δs between the actions of the two orbits is normally still small, and it is therefore more appropriate to start from the Berry-Tabor formula for semiclassical quantization in that regime than from Gutzwiller's trace formula, which assumes well-isolated periodic orbits. It is also important to note that the Berry-Tabor formula does not require an extensive numerical periodic orbit search. The periodic orbit parameters s/M_2 and g_E'' are smooth functions of the rotation number M_2/M_1, and can be obtained for arbitrary periodic orbits with coprime integers (M_1, M_2) by interpolation between "simple" rational numbers M_2/M_1.

We now demonstrate the high quality of the extension of Eqs. 1 and 2 to pairs of inverse hyperbolic and hyperbolic periodic orbits for a physical system that undergoes a transition from regularity to chaos, namely the hydrogen atom in a magnetic field. This is a scaling system, with $w = \gamma^{-1/3} = \hbar_{\mathrm{eff}}^{-1}$ the scaling parameter and $\gamma = B/(2.35 \times 10^5 \, \mathrm{T})$ the magnetic field strength in atomic units. Introducing scaled coordinates $\gamma^{2/3}\mathbf{r}$ and momenta $\gamma^{-1/3}\mathbf{p}$ and choosing the projection of the angular momentum on the magnetic field axis $L_z = 0$ one arrives at the scaled Hamiltonian

$$\tilde{H} = \frac{1}{2}\mathbf{p}^2 - \frac{1}{r} + \frac{1}{8}(x^2 + y^2) = \tilde{E} , \quad (5)$$

with $\tilde{E} = E\gamma^{-2/3}$ the scaled energy. At low energies $\tilde{E} < -0.6$ a Poincaré surface of section analysis of the classical dynamics [13] exhibits two different torus structures related to a "rotator" and "vibrator" type motion. The separatrix between these tori is destroyed at a scaled energy of $\tilde{E} \approx -0.6$, and the chaotic region around the separatrix grows with increasing energy. At $\tilde{E} = -0.127$ the classical phase space becomes completely chaotic. We investigate the system at scaled energy $\tilde{E} = -0.4$, where about 40% of the classical phase space volume is chaotic (see inset in Fig. 1), i.e. well in the region of mixed dynamics. We use 8 pairs of periodic orbits to describe the rotator type motion in both the regular and chaotic region. The results for the periodic orbit parameters $s/2\pi M_2$ and g_E'' are presented as solid lines in Fig. 1. The squares on the solid lines mark parameters obtained by pairs of stable and unstable periodic orbits in the regular region of the phase space. The diamonds mark parameters obtained by pairs of two unstable (inverse hyperbolic and hyperbolic) periodic orbits in the chaotic region of phase space. The cutoff is related to the winding angle $\phi = 1.278$ of the fixed point of the rotator type motion, i.e., the orbit perpendicular to the magnetic field axis, $(M_2/M_1)_{\mathrm{cutoff}} = \pi/\phi = 2.458$. The solid lines have been obtained by spline interpolation of the data points. In the same way the periodic orbit parameters for the vibrator type motion have been obtained from 11 pairs of periodic orbits (see the dashed lines in Fig. 1). The cutoff at $M_2/M_1 = \pi/\phi = 1.158$ is related to the winding angle $\phi = 2.714$ of the fixed point of the vibrator type motion, i.e., the orbit parallel to the field axis.

With the data of Fig. 1 we have all the ingredients at hand to calculate the semiclassical density of states $\varrho(w)$ in Eq. 1. The periodic orbit sum includes for both the rotator and vibrator type motion the orbits with $M_2/M_1 > (M_2/M_1)_{\mathrm{cutoff}}$. For each orbit the action and
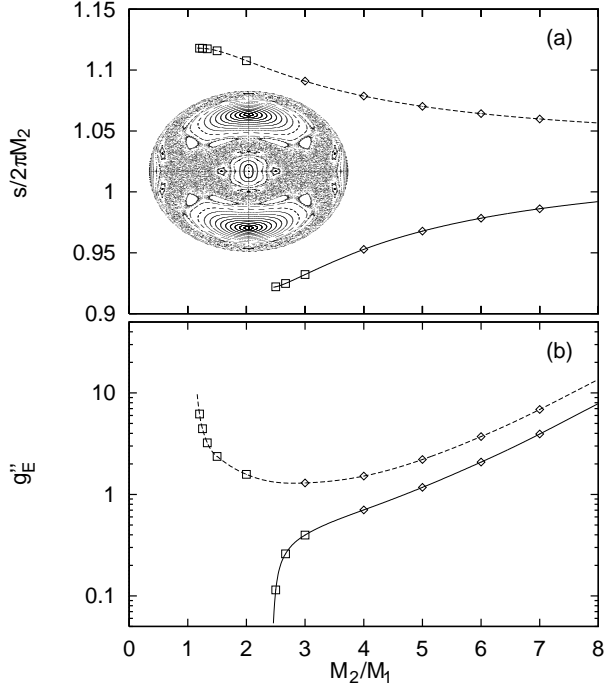
FIG. 1. (a) Action $s/2\pi M_2$ and (b) second derivative g_E'' as a function of the frequency ratio M_2/M_1 for the rotator (solid lines) and vibrator (dashed lines) type motion of the hydrogen atom in a magnetic field at scaled energy $\tilde{E} = -0.4$. Inset: Poincaré surface of section in semiparabolical coordinates $(\mu, p_\mu; \nu = 0)$.

the function g_E'' is obtained from the spline interpolations. The Maslov indices are $\eta_{\mathbf{M}} = 4M_2 - M_1$ for the rotator and $\eta_{\mathbf{M}} = 4M_2 + 2M_1 - 1$ for the vibrator type orbits. However, the problem is to extract the semiclassical eigenenergies from Eq. 1 because the periodic orbit sum does not converge. We therefore adopt the method of Refs. [16,17] where we proposed to adjust the semiclassical recurrence signal, i.e., the Fourier transform of the weighted density of states $w^{-1/2}\varrho(w)$ (Eq. 1)

$$C^{\mathrm{sc}}(s) = \sum_{\mathbf{M}} \mathcal{A}_{\mathbf{M}} \delta(s - s_{\mathbf{M}}) , \qquad (6)$$

with the amplitudes being determined exclusively by periodic orbit quantities,

$$\mathcal{A}_{\mathbf{M}} = \frac{s_{\mathbf{M}}}{M_2^{3/2} |g_E''|^{1/2}} \, e^{-i\frac{\pi}{2}\eta_{\mathbf{M}}} , \qquad (7)$$

to the functional form of its quantum mechanical analogue

$$C^{\mathrm{qm}}(s) = -i \sum_k d_k e^{-iw_k s} , \qquad (8)$$

where the w_k are the quantum eigenvalues of the scaling parameter, and the d_k are the multiplicities of the
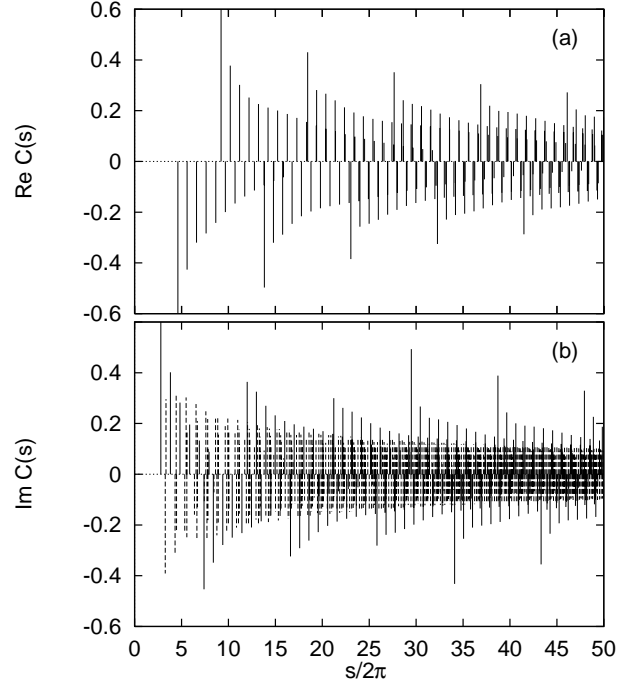

FIG. 2. Semiclassical recurrence signal $C^{\mathrm{sc}}(s)$ for the hydrogen atom in a magnetic field at scaled energy $\tilde{E} = -0.4$. Solid and dashed sticks: Signal from the rotator and vibrator type motion, respectively.

eigenvalues ($d_k = 1$ for nondegenerate states). The frequencies obtained from this procedure are interpreted as the semiclassical eigenvalues w_k. The technique used to adjust (6) to (8) is harmonic inversion [17].

For the hydrogen atom in a magnetic field part of the semiclassical recurrence signal $C^{\mathrm{sc}}(s)$ at scaled energy $\tilde{E} = -0.4$ is presented in Fig. 2. The solid and dashed peaks mark the recurrencies of the rotator and vibrator type orbits, respectively. Note that $C^{\mathrm{sc}}(s)$ can be easily calculated even for long periods s with the help of the spline interpolation functions in Fig. 1. By contrast, the construction of the recurrence signal for Gutzwiller's trace formula usually requires an exponentially increasing effort for the numerical periodic orbit search with growing period.

We have analyzed $C^{\mathrm{sc}}(s)$ by the harmonic inversion technique in the region $0 < s/2\pi < 200$. The resulting semiclassical spectrum of the lowest 106 states with eigenvalues $w < 20$ is shown in the upper part of Fig. 3a. For graphical purposes the spectrum is presented as a function of the squared scaling parameter w^2, which is equivalent to unfolding the spectrum to constant mean level spacing. For comparison the lower part of Fig. 3a shows the exact quantum spectrum. The semiclassical and quantum spectrum are seen to be in excellent agreement, and deviations are less than the stick widths for nearly all states. The distribution $P(d)$ of the semiclassical error with $d = (w_{\mathrm{qm}} - w_{\mathrm{sc}})/\Delta w_{\mathrm{av}}$ the error in units
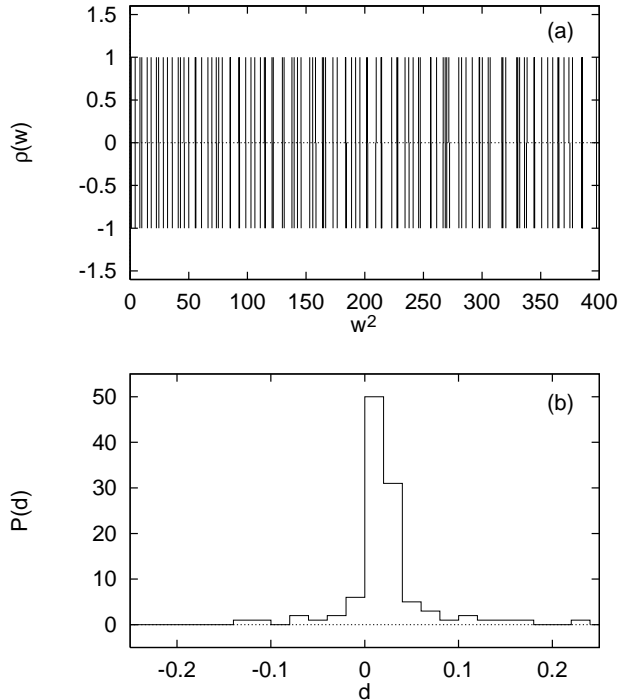
FIG. 3. (a) Semiclassical and quantum mechanical spectrum of the hydrogen atom in a magnetic field at scaled energy $\tilde{E} = -0.4$. (b) Distribution $P(d)$ of the semiclassical error in units of the mean level spacing, $d = (w_{qm} - w_{sc})/\Delta w_{av}$ for the lowest 106 eigenvalues.

of the mean level spacing, $\Delta w_{av} = 1.937/w$, is presented in Fig. 3b. For most levels the semiclassical error is less than 4% of the mean level spacing, which is typical for a system with two degrees of freedom [18].

The accuracy of the results presented in Fig. 3 seems to be surprising for two reasons. First, we have not exploited the mean staircase function $\bar{N}(w)$, i.e., the number of eigenvalues w_k with $w_k < w$, which is a basic requirement of some other semiclassical quantization techniques for bound chaotic systems [5,6]. Second, as mentioned before, Eq. 2 has been derived for near-integrable systems, and is only an approximation, in particular, for mixed systems. We have not taken into account any more refined extensions of the Berry-Tabor formula (1) as discussed, e.g., in Ref. [11]. The answer to the second point is that the splitting of scaled actions of the periodic orbit pairs used in Fig. 1 does not exceed $\Delta s = 0.022$, and therefore for states with $w < 20$ the phase shift between the two periodic orbit contributions is $w\Delta s = 0.44$, at most. For small phase shifts the extension of the Berry-Tabor formula to near-integrable systems results in a damping of the *amplitudes* of the periodic orbit recurrence signal in Fig. 2 but seems not to effect the *frequencies*, i.e., the semiclassical eigenvalues w_k obtained by the harmonic inversion of the function $C^{sc}(s)$.

In conclusion, we have presented a solution to the fundamental problem of semiclassical quantization of non-integrable systems in the mixed regular-chaotic regime. We have demonstrated the excellent quality of our procedure for the hydrogen atom in a magnetic field at a scaled energy $\tilde{E} = -0.4$, where about 40% of the phase space volume is chaotic. The lowest 106 semiclassical and quantum eigenenergies have been shown to agree within a few percent of the mean level spacings. Obviously, it will be straightforward, and rewarding, to apply the method to other systems with mixed dynamics.

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